

Message

From: Chandramouli, Bharat (Sidney) [Bharat.Chandramouli@sgs.com]
Sent: 8/27/2019 4:11:11 PM
To: Strynar, Mark [/o=ExchangeLabs/ou=Exchange Administrative Group (FYDIBOHF23SPDLT)/cn=Recipients/cn=5a9910d5b38e471497bd875fd329a20a-Strynar, Mark]
CC: McCord, James [/o=ExchangeLabs/ou=Exchange Administrative Group (FYDIBOHF23SPDLT)/cn=Recipients/cn=McCord, James]
Subject: RE: [EXTERNAL] RE: Following up on Solvay Product and PFOS interference Q

Mark:

This is super helpful, thanks so much

Bharat

From: Strynar, Mark <Strynar.Mark@epa.gov>
Sent: August 27, 2019 7:25 AM
To: Chandramouli, Bharat (Sidney) <Bharat.Chandramouli@sgs.com>
Cc: McCord, James <mccord.james@epa.gov>
Subject: [EXTERNAL] RE: Following up on Solvay Product and PFOS interference Q

*** WARNING: this message is from an EXTERNAL SENDER. Please be cautious, particularly with links and attachments. ***

Sidney,

For the NJ DEP work around the Solvay plant we have seen a suite of these CI-PFECAs with the most abundant peak being the chemical we call CI PFECA 1,0 for the 1 propyl 0 ethyl linkage in the middle. See the attached slides. This naming convention comes from the Wang et al., 2013 paper cited in slide #4. I can say for sure we did the MS/MS on our Orbitrap for at least this one. I cannot say for the others.

A couple of items to note:

- 1) They do not decarboxylate like other PFCAs, the linkage breaks at the first ether near the carboxylate (see slide 3) and you lose C2 F2 O3 H
- 2) They all have the C3 F6 Cl O tail m/z 200.9537 in slide 3. We draw it as linear, however we really don't know if it is linear or branched.

As far as the PFOS interferent in the AFFF samples, we did not follow-up to try to figure out what it was as I recall. Simply that it was not PFOS. James may have more to add to all of this so I am cc'ing him. If you use HRMS you would see this also, but I don't recall what sample we even did this on. I think in all of these instances for QQQ work on PFOS in particular ion ratios of 499-99 and 499-80 are essential. I would even perhaps throw in a 3rd MRM if possible.

Cheers,
Mark

From: Chandramouli, Bharat (Sidney) <Bharat.Chandramouli@sgs.com>
Sent: Monday, August 26, 2019 1:37 PM

To: Strynar, Mark <Strynar.Mark@epa.gov>

Subject: Following up on Solvay Product and PFOS interference Q

Hello Mark:

Always a pleasure running into you at a conference, gold mine of information. If you need a peer-reviewer on your PFAS lessons learned paper, feel free to suggest my name.

Following up on our conversation on the Solvay product, Sandra Goodrow of the NJDEP reached out to us wanting some help in at least a semi-quantitative estimation of the major constituents of waste from the Solvay fluoropolymer manufacture process. She mentioned you'd done some initial HRMS work on these samples. As we discussed, we have some options to proceed on:

- 1) If you had some precursor—product information based on MS/MS type experiments that you're able to share, that would enable us to move forward fairly easily. At present, only the major constituent is of interest, but others depending on abundance may be on the radar as well
- 2) If you were not able to do MS/MS experiments, at least a molecular ion, scan data and a putative structure would be handy. As you mentioned, we maybe able to infuse a high-abundance sample at the last resort.

Let me know if you're able to help and I'll get back in touch with Sandra about this.

Also, at the conference, Janis mentioned you had done a HRMS scan on a sample with a PFOS interference and got a suspect sulfonate. Do you have any more info on this you're able to share? A client of ours with some strange PFOS data on a project would like to rule out an interference.

Thanks in advance.

Bharat Chandramouli, Ph. D
Environment, Health and Safety
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